

L7 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2009 ACS on STN

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DOCUMENT NUMBER: 139:230770

TITLE: 5-Phenylthiazole derivatives and their use as
phosphatidylinositol 3-kinase (Pi3K) inhibitors for
the treatment of allergic and inflammatory diseasesINVENTOR(S): Bruce, Ian; Finan, Peter; Leblanc, Catherine;
McCarthy, Clive; Whitehead, Lewis; Blair, Nicola
Elaine; Bloomfield, Graham Charles; Hayler, Judy;
Kirman, Louise; Oza, Mrinalini Sachin; Shukla, Lena
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.

SOURCE: PCT Int. Appl., 101 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

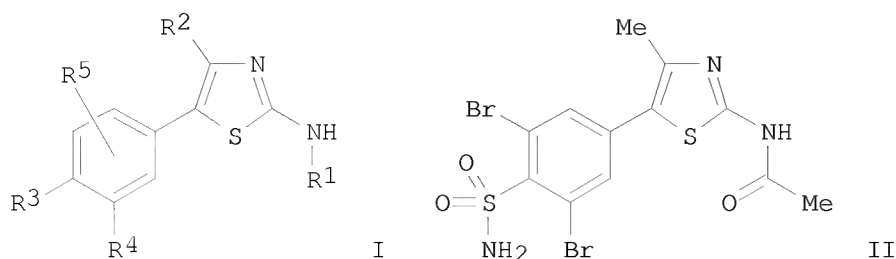
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072557	A1	20030904	WO 2003-EP2036	20030227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SE, SG, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR				
CA 2477601	A1	20030904	CA 2003-2477601	20030227
AU 2003214080	A1	20030909	AU 2003-214080	20030227
EP 1480962	A1	20041201	EP 2003-709730	20030227
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008030	A	20041228	BR 2003-8030	20030227
CN 1639139	A	20050713	CN 2003-804796	20030227
JP 2005522458	T	20050728	JP 2003-571263	20030227
NZ 534657	A	20070531	NZ 2003-534657	20030227
IN 2004CN01872	A	20060623	IN 2004-CN1872	20040823
MX 2004008362	A	20041126	MX 2004-8362	20040827
NO 2004004095	A	20041102	NO 2004-4095	20040927
US 20050119320	A1	20050602	US 2005-504259	20050131
ZA 2004006292	A	20060531	ZA 2004-6292	20060320
AU 2007203160	A1	20070726	AU 2007-203160	20070706
PRIORITY APPLN. INFO.:			GB 2002-4765	A 20020228
			GB 2002-29626	A 20021219
			AU 2003-214080	A3 20030227
			WO 2003-EP2036	W 20030227

OTHER SOURCE(S): MARPAT 139:230770

GI



AB Title compds. I, in free or salt form, are disclosed [wherein: R1 = H, aminocarbonyl optionally substituted by nitrile, or alkylcarbonyl, alkylaminocarbonyl, heterocyclylaminocarbonyl, heterocyclylcarbonyl, benzoyl, phenylaminocarbonyl, cycloalkanoyl, or cycloalkylaminocarbonyl, all of which are optionally substituted by a wide variety of groups; R2 = C1-3 alkyl or halogen; one of R3 and R4 = R6 and the other = R7; R5 = H or halo; R6 = H, OH, amino, -SOR8, -SO2R8, -SO2NH2, -SO2NR9R10, -COR8, -CONHR8, -NHSO2R8, nitrile, carboxy, -OR8 or haloalkyl; R7 = H, R11, -OR11, halo, carboxy, -SO2R8, cyano, or haloalkyl, or, when R4 = R7, R7 can also = -NR12R13, R14, or -OR14; R8, R11 = (un)substituted alkyl or cycloalkyl; either R9 = alkyl or cycloalkyl, optionally substituted by OH, alkoxy, nitrile, amino, alkylamino, dialkylamino, or a 5- or 6-membered N/O/S-heterocyclyl optionally substituted by alkyl; and R10 = H or alkyl; or NR9R10 = 5- or 6-membered N/O/S-heterocyclyl optionally substituted by alkyl; either R12 = alkyl or cycloalkyl optionally substituted by hydroxy, amino, alkylamino or dialkylamino; and R13 = H or alkyl; or NR12R13 = 5- or 6-membered N/O/S-heterocyclyl optionally substituted by alkyl; R14 = alkyl optionally substituted by hydroxy or -NR12R13]. I are useful for treating diseases mediated by phosphatidylinositol 3-kinase (Pi3K), particularly the gamma isoform (p110 γ). Pharmaceutical compns. that contain the compds. and processes for preparing the compds. are also described. Approx. 180 specific examples are described and claimed. For instance, N-[4-methyl-5-(4-nitrophenyl)thiazol-2-yl]acetamide underwent a sequence of: (1) hydrogenation of nitro to amino over Pd/C; (2) 3,5-dibromination of the 4-aminophenyl ring using Br₂ in 1,4-dioxane; (3) diazotization of the amine; (4) chlorosulfonylation of the diazonium salt with SO₂ and CuCl₂ in aqueous HCl/AcOH; and (5) ammonolysis of the resultant sulfonyl chloride with NH₃ and Na₂CO₃ in dioxane, to give invention compound II. In an in vitro assay against human recombinant Pi3K γ expressed by Sf9 insect cells, I had IC₅₀ values below 0.6 μ M in an in vitro assay. Several example compds. had IC₅₀ values in the range of 0.002-0.040 μ M, including II (0.009 μ M).

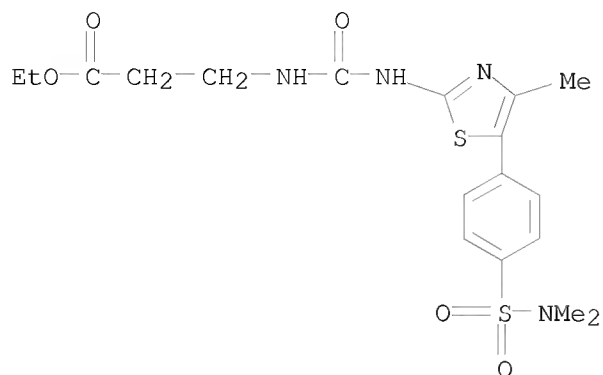
IT **593958-80-6P**, 3-[3-[5-(4-Dimethylsulfamoylphenyl)-4-methylthiazol-2-yl]ureido]propionic acid ethyl ester **593959-15-0P**, [3-[5-[4-(Methanesulfonyl)phenyl]-4-methylthiazol-2-yl]ureido]acetic acid ethyl ester **593960-33-9P**, 1-[2-(5-Ethylloxazol-2-yl)ethyl]-3-[5-[3-fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]urea

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of phenylthiazole derivs. as
phosphatidylinositol 3-kinase inhibitors)

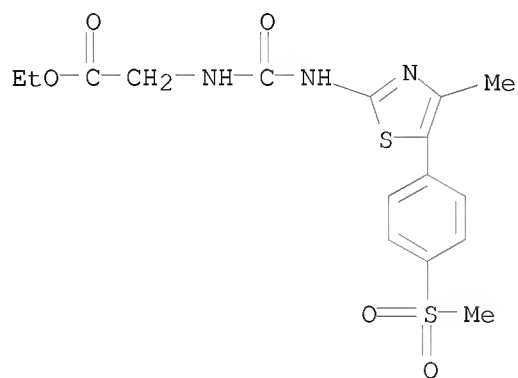
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CN β -Alanine, N-[[[5-[4-[(dimethylamino)sulfonyl]phenyl]-4-methyl-2-thiazolyl]amino]carbonyl]-, ethyl ester (CA INDEX NAME)



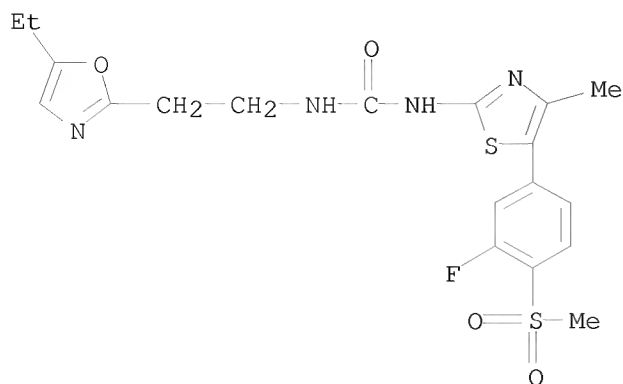
RN 593959-15-0 ZCAPLUS

CN Glycine, N-[[[4-methyl-5-[4-(methylsulfonyl)phenyl]-2-thiazolyl]amino]carbonyl]-, ethyl ester (CA INDEX NAME)



RN 593960-33-9 ZCAPLUS

CN Urea, N-[2-(5-ethyl-2-oxazolyl)ethyl]-N'-[5-[3-fluoro-4-(methylsulfonyl)phenyl]-4-methyl-2-thiazolyl]- (CA INDEX NAME)



IT **593958-79-3P**, [3-[5-(4-Dimethylsulfamoylphenyl)-4-methylthiazol-2-yl]ureido]acetic acid ethyl ester **593959-16-1P**, [3-[5-[4-(Methanesulfonyl)phenyl]-4-methylthiazol-2-yl]ureido]acetic acid **593959-17-2P**, 3-[3-[5-[4-(Methanesulfonyl)phenyl]-4-methylthiazol-2-yl]ureido]propionic acid **593959-43-4P**, 1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(2-hydroxyethyl)urea **593959-44-5P**, 1-(2-Cyanoethyl)-3-[5-[3-fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]urea **593959-46-7P**, 1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(3-hydroxypropyl)urea **593959-47-8P**, 1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(pyridin-2-yl)methyl]urea **593959-48-9P**, 1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[2-(pyridin-2-yl)ethyl]urea **593959-49-0P**, 1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[2-(pyridin-3-yl)ethyl]urea **593959-51-4P**, 1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(4-hydroxybutyl)urea **593959-54-7P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(furan-2-yl)methyl]urea **593959-55-8P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(2-cyanoethyl)urea **593959-56-9P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(2,5-dimethyl-2H-pyrazol-3-yl)urea **593959-60-5P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(pyridin-2-yl)methyl]urea **593959-64-9P**, Azetidine-1-carboxylic acid [5-[4-chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide **593959-65-0P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(pyridin-4-yl)methyl]urea **593959-66-1P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(pyridin-3-yl)methyl]urea **593959-67-2P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[3-(imidazol-1-yl)propyl]urea **593959-68-3P**, Pyrrolidine-1-carboxylic acid [5-[4-chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide **593959-70-7P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[2-(1-methylpyrrolidin-2-yl)ethyl]urea **593959-71-8P**, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(furan-3-

ylmethyl)urea 593959-72-9P,
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1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(S)-1-(hydroxymethyl)propyl]urea 593959-76-3P,
1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-((R)-2-hydroxy-1-methylethyl)urea 593959-77-4P,
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1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[2-(2-hydroxyethoxy)ethyl]urea 593959-79-6P,
1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[3-(diethylamino)propyl]urea 593959-80-9P,
1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(pyridin-3-yl)urea 593959-81-0P, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(pyridin-4-yl)urea 593959-82-1P, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(2-methyl-2H-pyrazol-3-yl)urea 593959-83-2P,
1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(1,3,5-trimethyl-1H-pyrazol-4-yl)urea 593959-84-3P,
1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[(5-methylisoxazol-3-yl)methyl]urea 593959-85-4P,
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1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-((S)-2-hydroxy-2-phenylethyl)urea 593959-90-1P,
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3-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-1-(2-hydroxyethyl)-1-methylurea 593959-96-7P,
(R)-3-Hydroxypyrrolidine-1-carboxylic acid
[5-[4-chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide 593959-97-8P, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(4-hydroxybutyl)urea 593959-98-9P,
1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-(5-hydroxypentyl)urea 593959-99-0P,
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1-(2-Cyanoethyl)-3-[5-[3-(imidazol-1-yl)-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]urea 593960-06-6P,
1-(3-Hydroxypropyl)-3-[5-[3-(imidazol-1-yl)-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]urea 593960-07-7P,
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1-(2-Cyanoethyl)-1-ethyl-3-[5-[3-(imidazol-1-yl)-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]urea 593960-17-9P,

3-Hydroxyazetidine-1-carboxylic acid

[5-[4-chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide

593960-18-0P, 1-[5-[4-Chloro-3-(methanesulfonyl)phenyl]-4-

methylthiazol-2-yl]-3-[6-(morpholin-4-yl)pyridin-3-yl]urea

593960-19-1P, 4-[3-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-

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3-[3-[5-[3-(Methanesulfonyl)phenyl]-4-methylthiazol-2-yl]ureido]propionic

acid ethyl ester **593960-34-0P**,

1-[2-(4-Ethylloxazol-2-yl)ethyl]-3-[5-[3-fluoro-4-(methanesulfonyl)phenyl]-

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1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[2-(5-

methyloxazol-2-yl)ethyl]urea **593960-36-2P**,

1-[5-[3-Fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]-3-[2-(4-

methyloxazol-2-yl)ethyl]urea

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

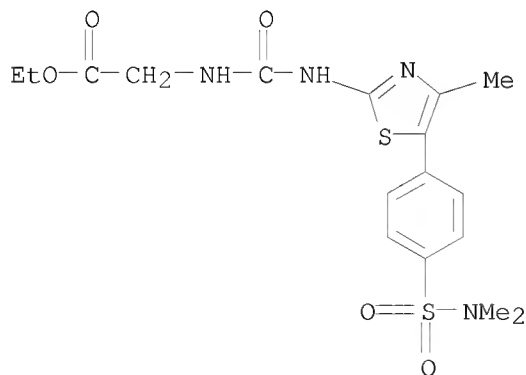
(Uses)

(drug candidate; preparation of phenylthiazole derivs. as

phosphatidylinositol 3-kinase inhibitors)

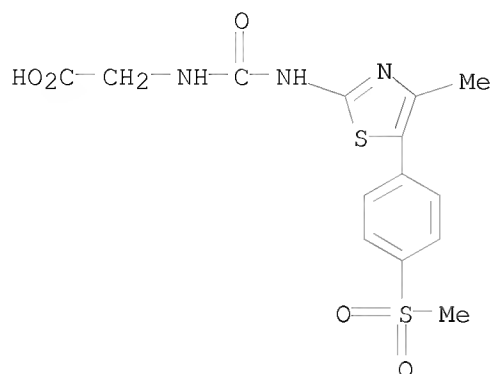
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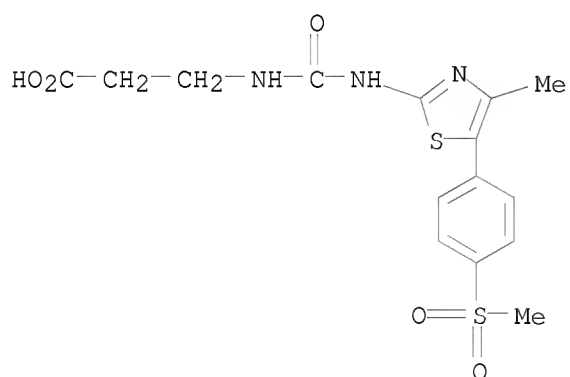
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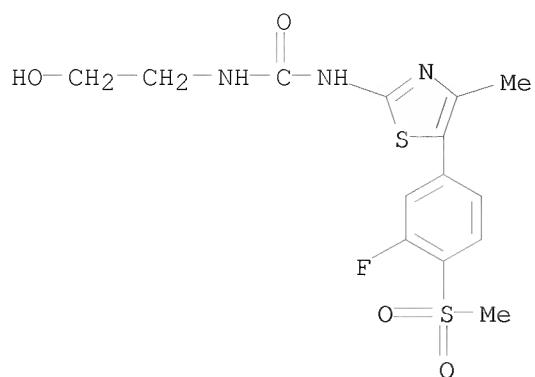
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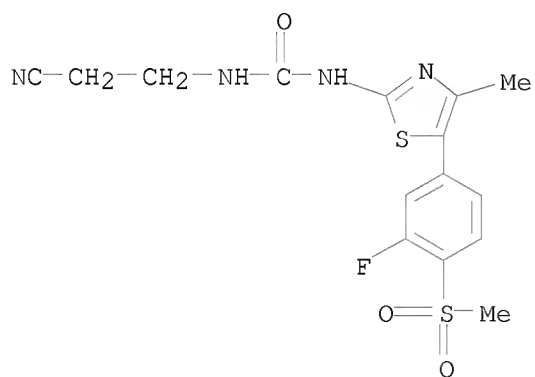
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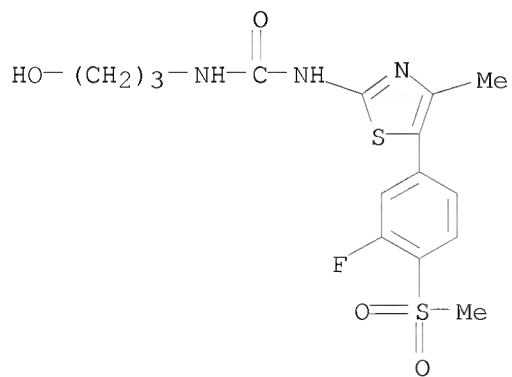
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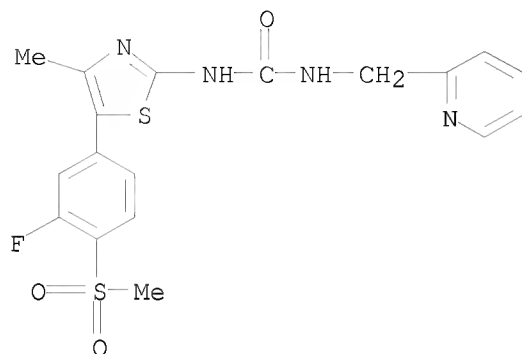
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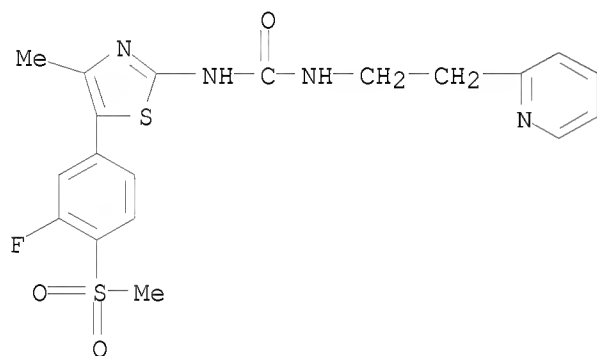
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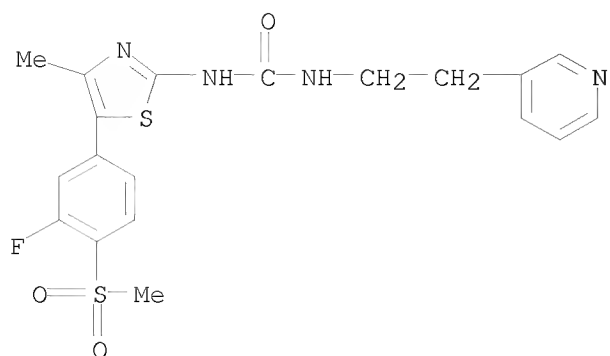
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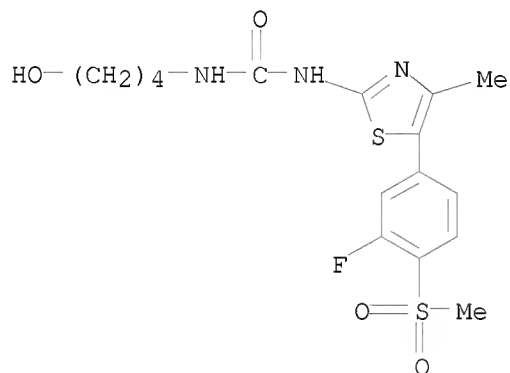
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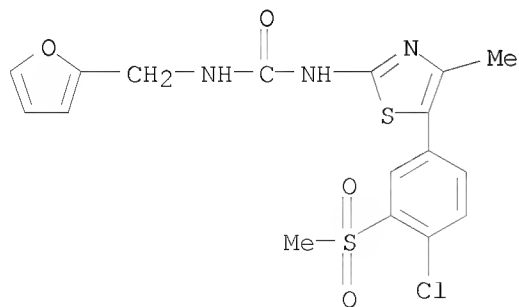
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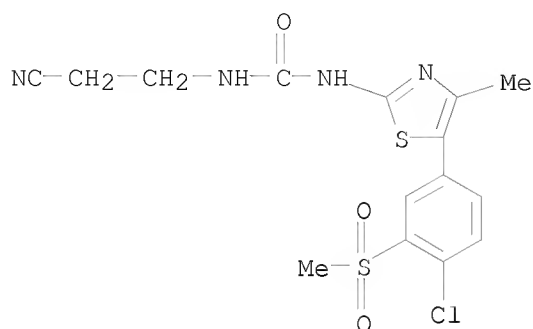
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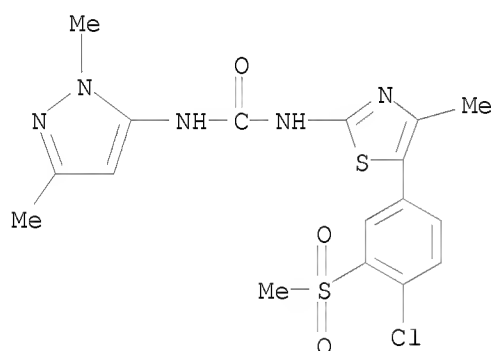
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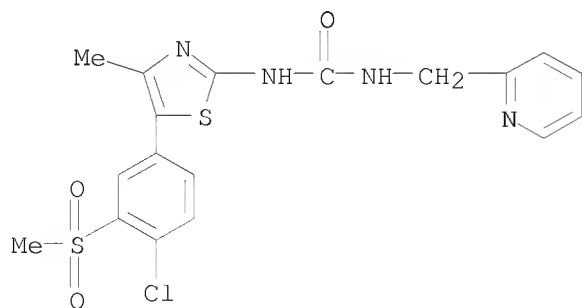
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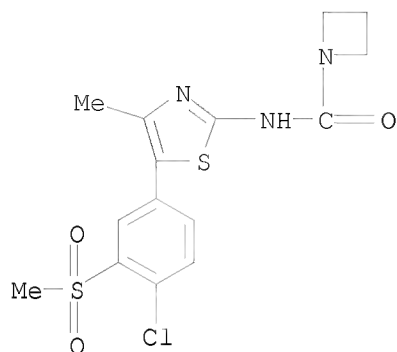
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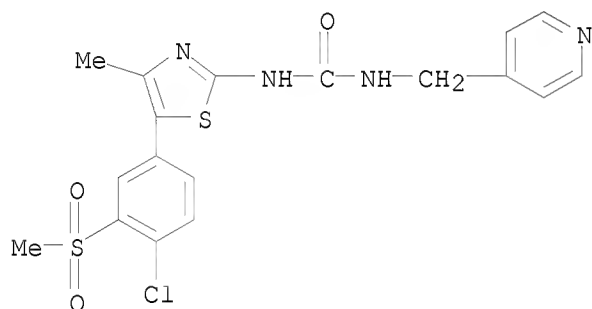
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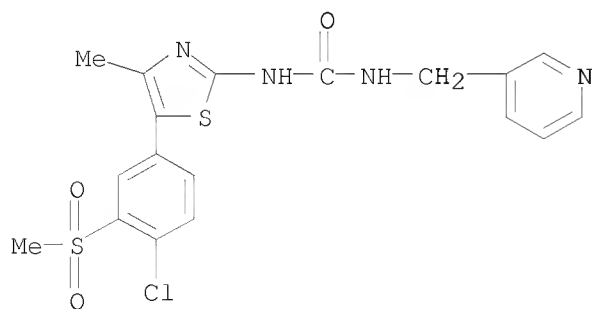
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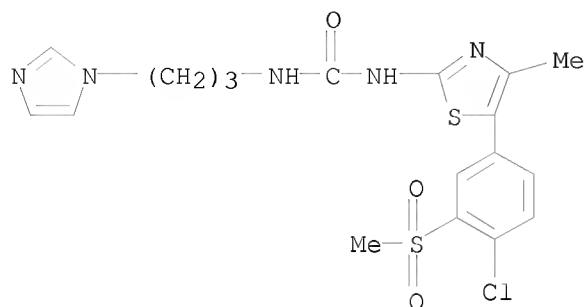
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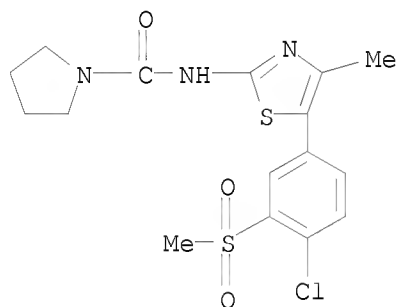
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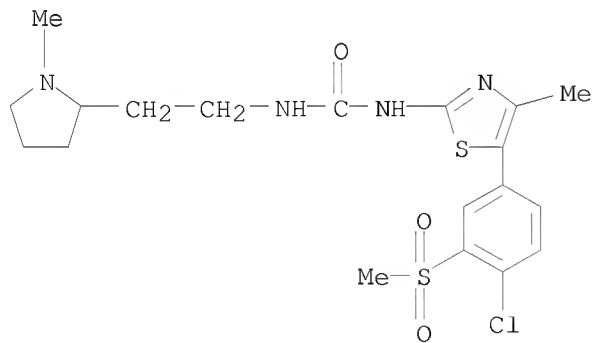
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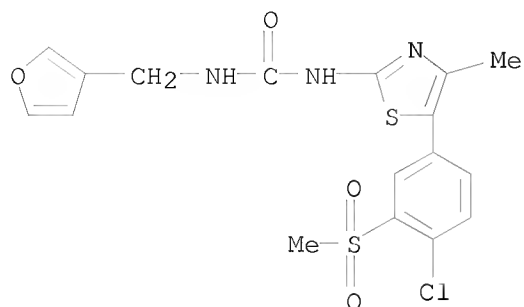
RN 593959-70-7 ZCAPLUS

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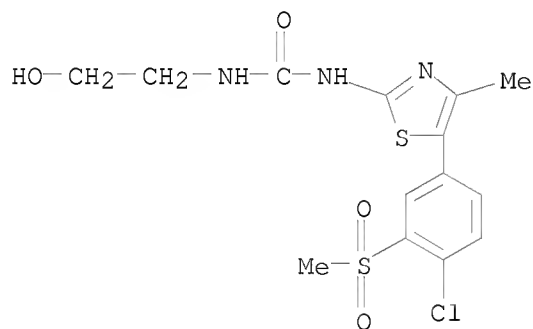
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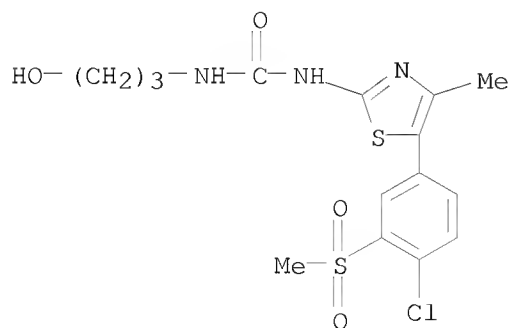
RN 593959-72-9 ZCAPLUS

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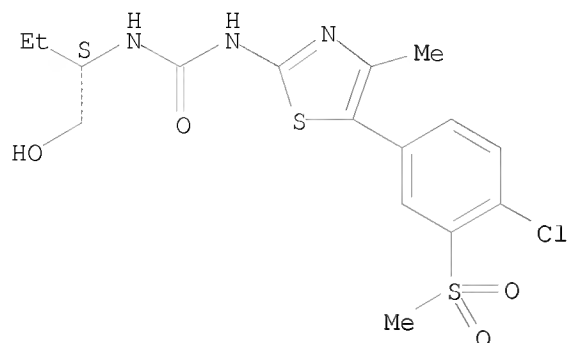
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RN 593959-74-1 ZCAPLUS

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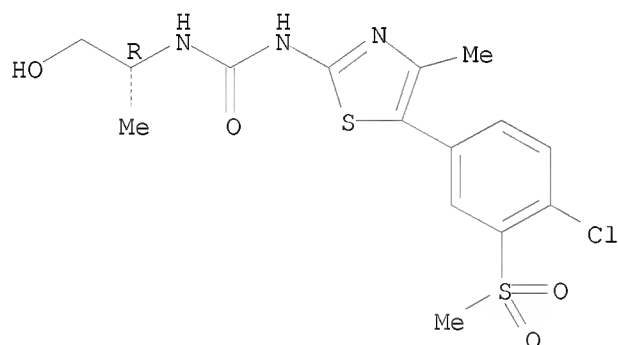
Absolute stereochemistry.



RN 593959-76-3 ZCAPLUS

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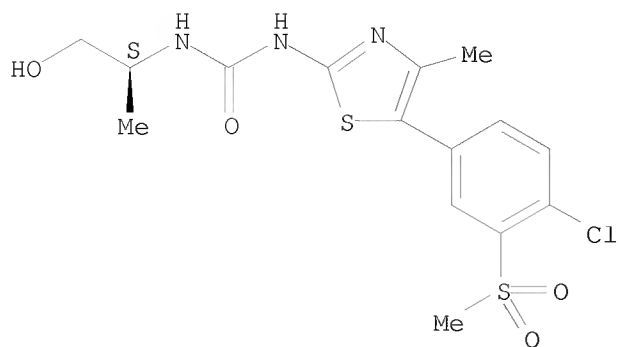
Absolute stereochemistry.



RN 593959-77-4 ZCAPLUS

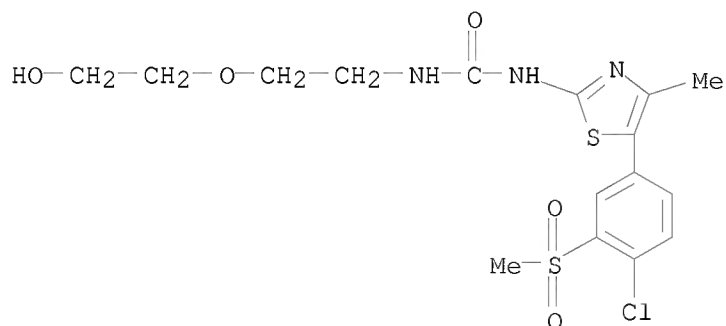
CN Urea, N-[5-[4-chloro-3-(methylsulfonyl)phenyl]-4-methyl-2-thiazolyl]-N'-[(1S)-2-hydroxy-1-methylethyl]- (CA INDEX NAME)

Absolute stereochemistry.



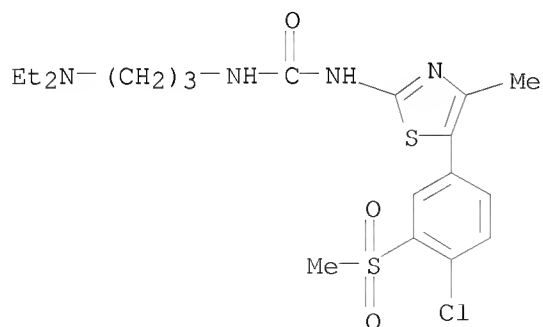
RN 593959-78-5 ZCAPLUS

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RN 593959-79-6 ZCAPLUS

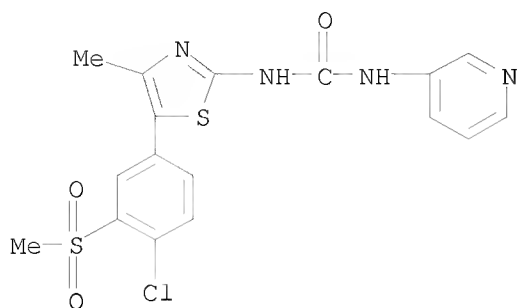
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RN 593959-80-9 ZCAPLUS

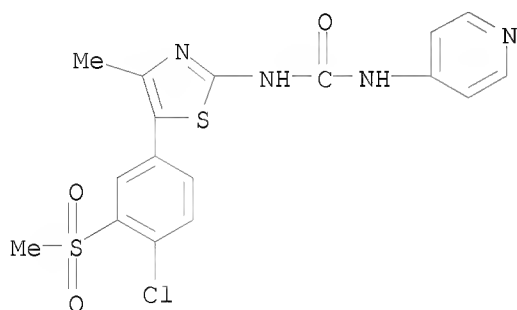
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pyridinyl- (CA INDEX NAME)



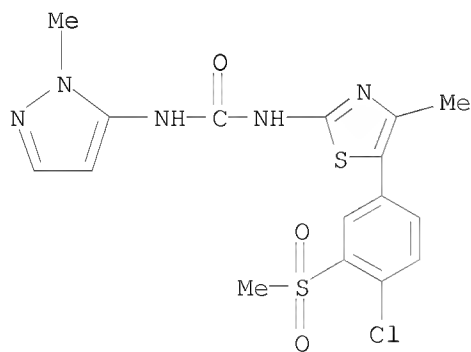
RN 593959-81-0 ZCAPLUS

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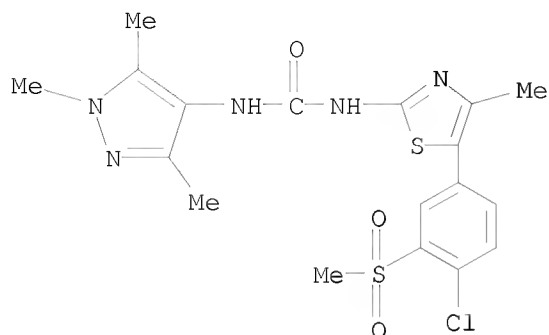
RN 593959-82-1 ZCAPLUS

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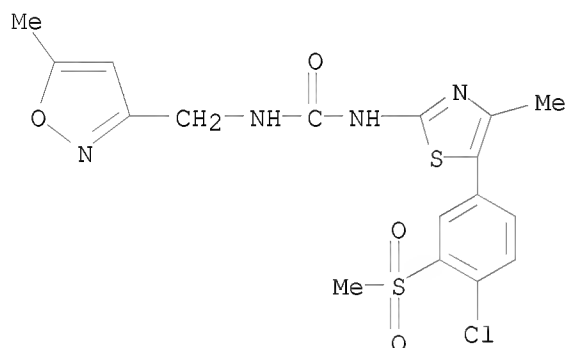
RN 593959-83-2 ZCAPLUS

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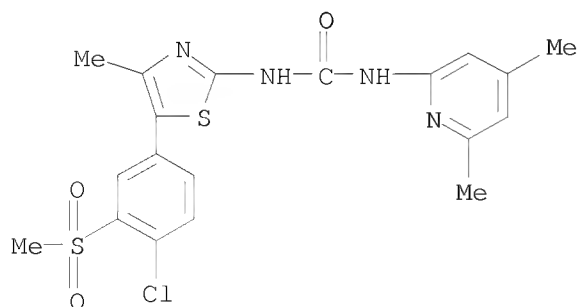
RN 593959-84-3 ZCAPLUS

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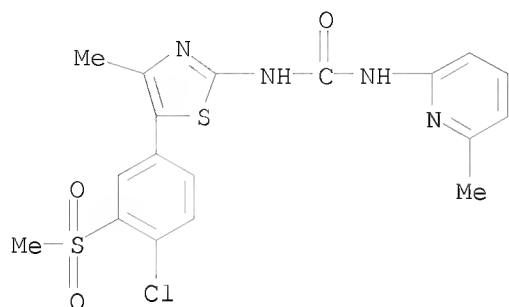
RN 593959-85-4 ZCAPLUS

CN Urea, N-[5-[4-chloro-3-(methylsulfonyl)phenyl]-4-methyl-2-thiazolyl]-N'-(4,6-dimethyl-2-pyridinyl)- (CA INDEX NAME)



RN 593959-86-5 ZCAPLUS

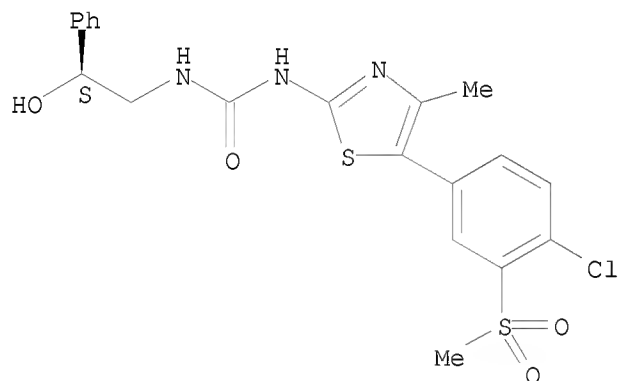
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RN 593959-87-6 ZCAPLUS

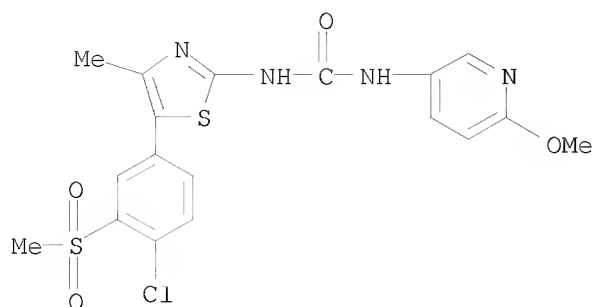
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Absolute stereochemistry.



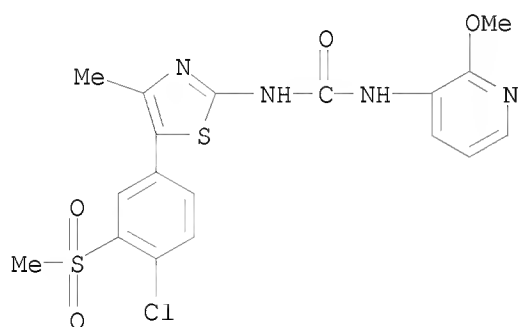
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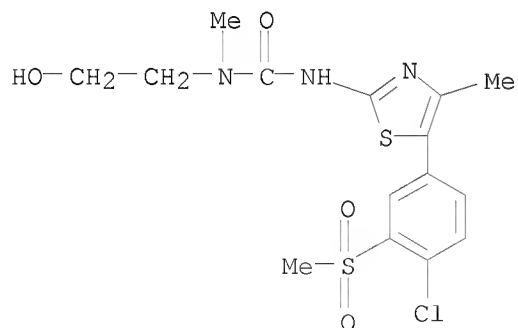
RN 593959-91-2 ZCAPLUS

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RN 593959-95-6 ZCAPLUS

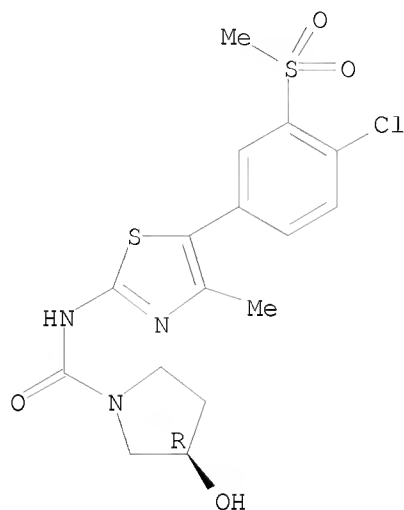
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RN 593959-96-7 ZCAPLUS

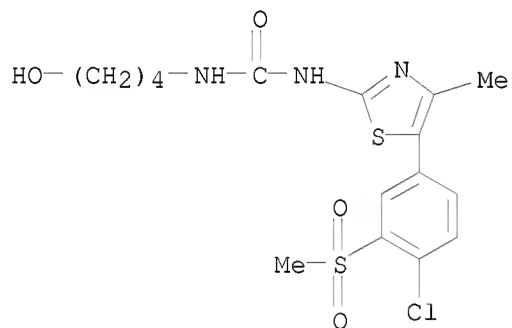
CN 1-Pyrrolidinecarboxamide, N-[5-[4-chloro-3-(methylsulfonyl)phenyl]-4-methyl-2-thiazolyl]-3-hydroxy-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



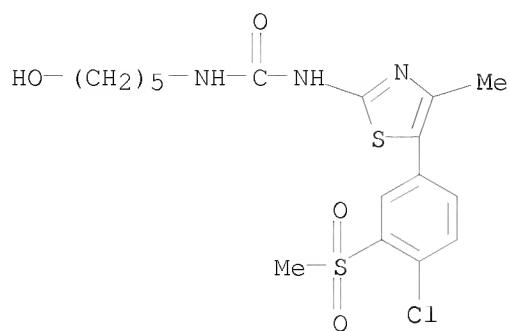
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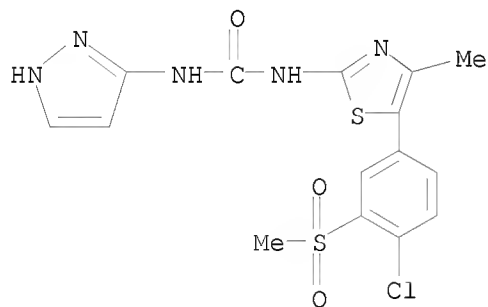
RN 593959-98-9 ZCAPLUS

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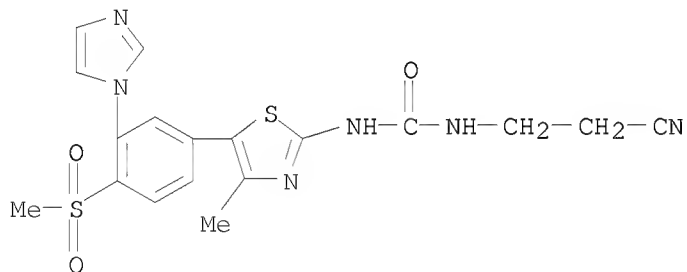
RN 593959-99-0 ZCAPLUS

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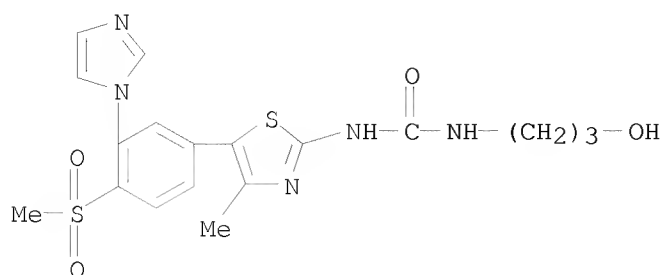
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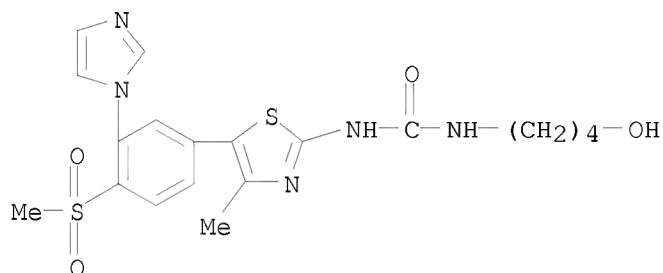
RN 593960-06-6 ZCAPLUS

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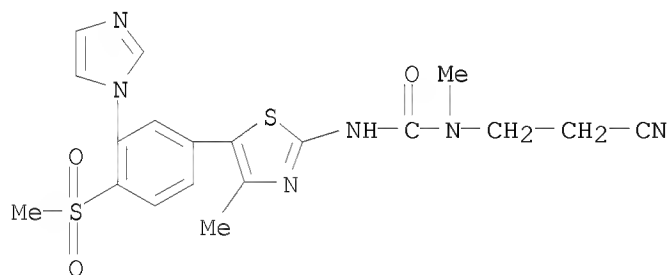
RN 593960-07-7 ZCAPLUS

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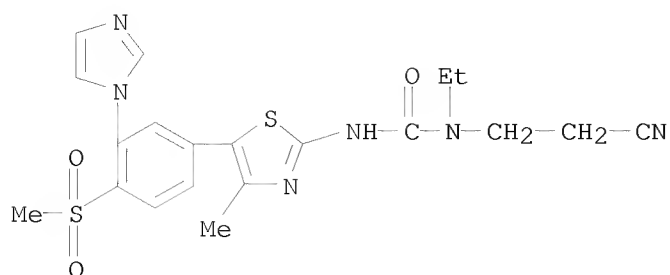
RN 593960-09-9 ZCAPLUS

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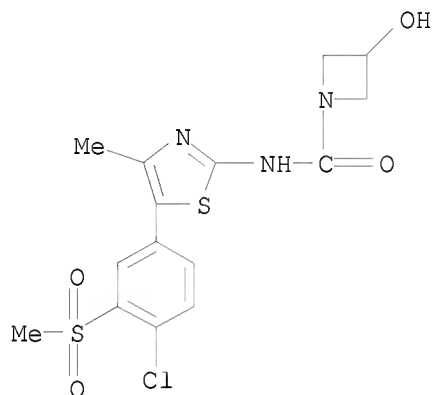
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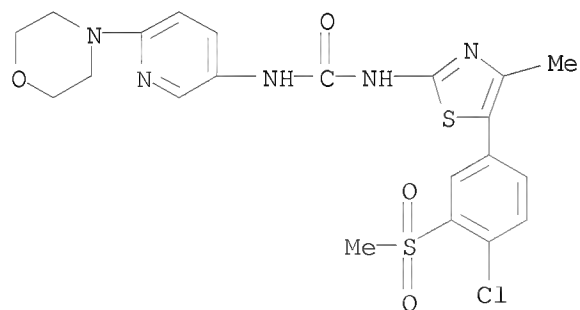
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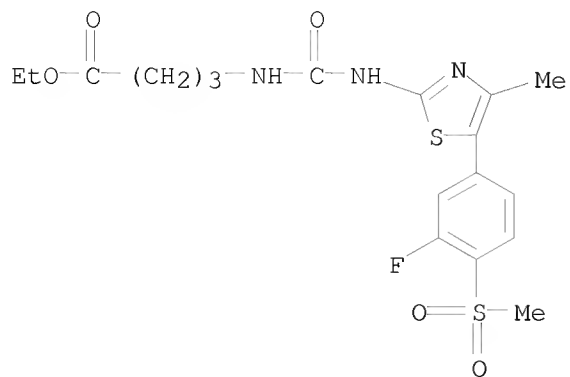
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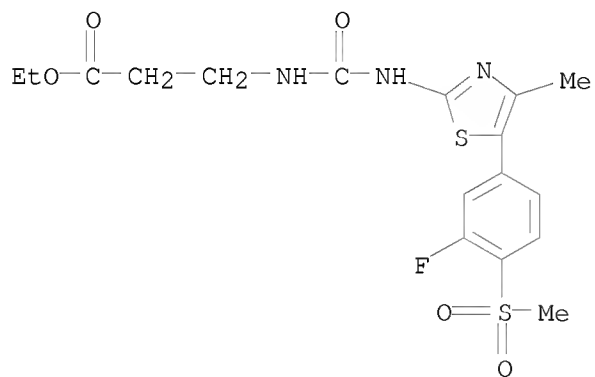
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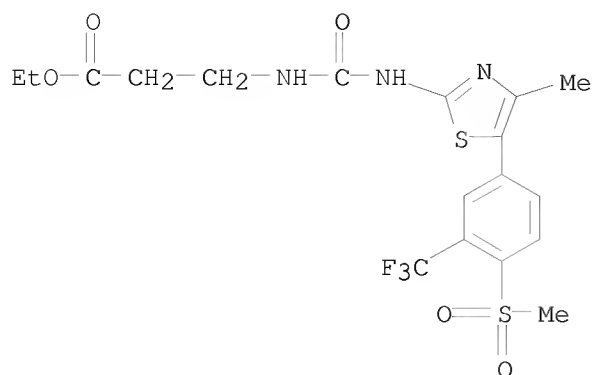
RN 593960-20-4 ZCAPLUS

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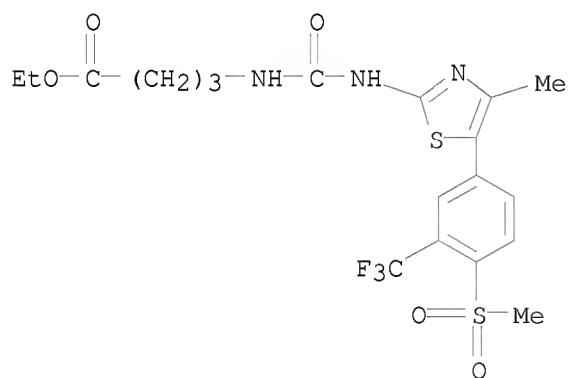
RN 593960-21-5 ZCAPLUS

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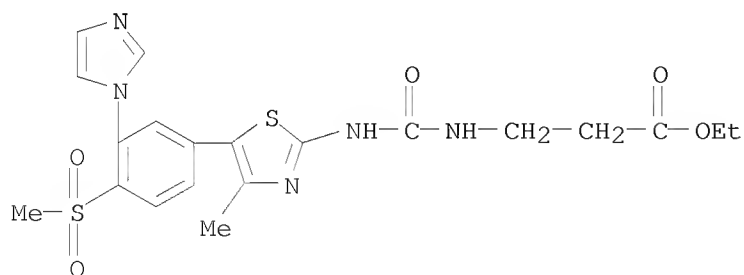
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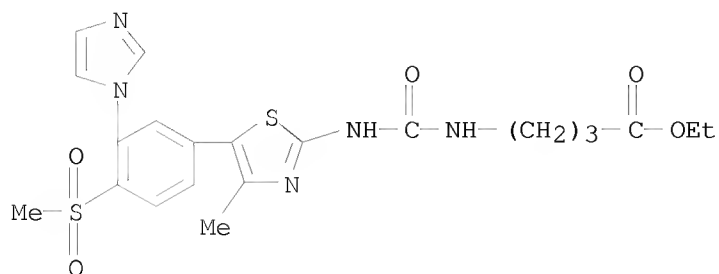
RN 593960-23-7 ZCAPLUS

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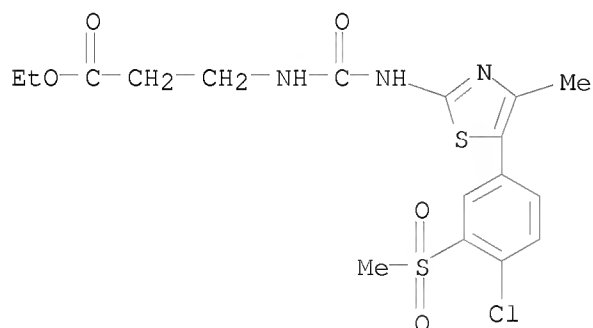
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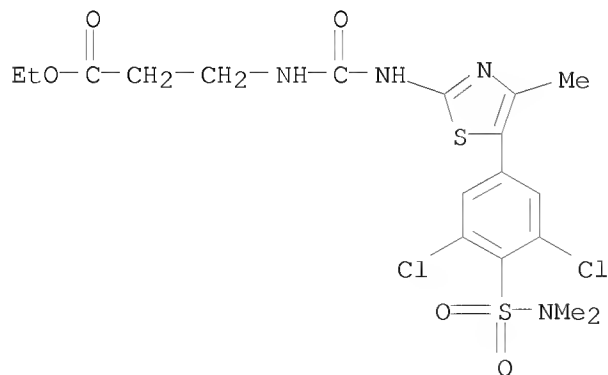
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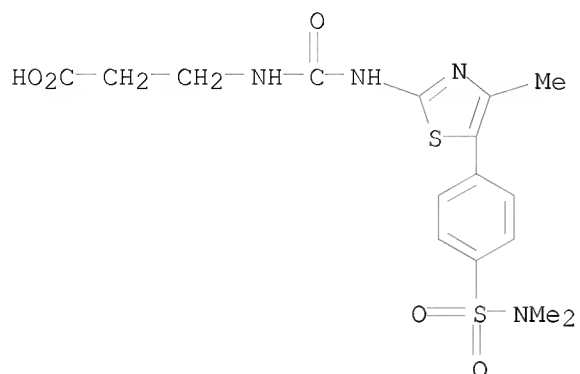


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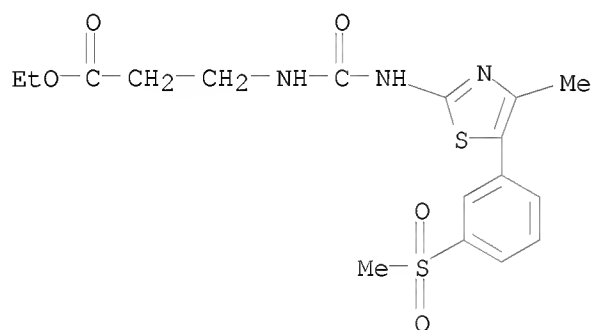
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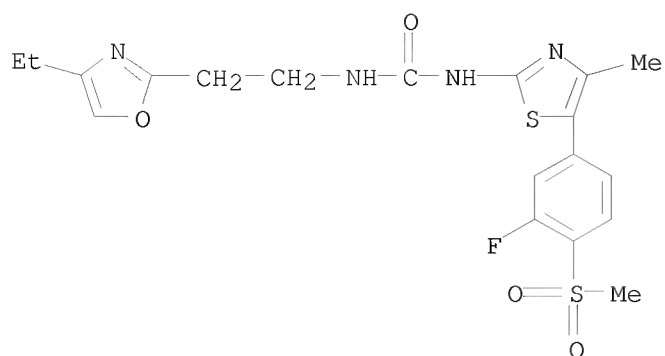
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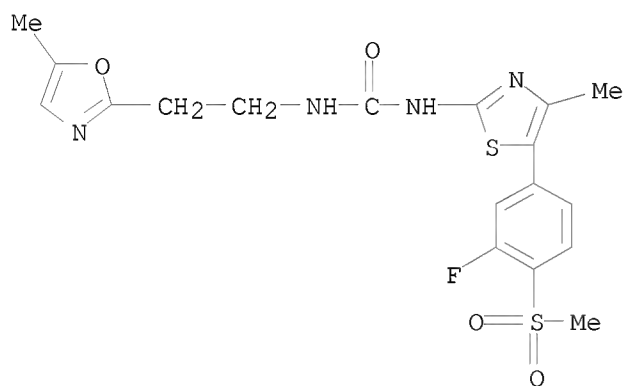
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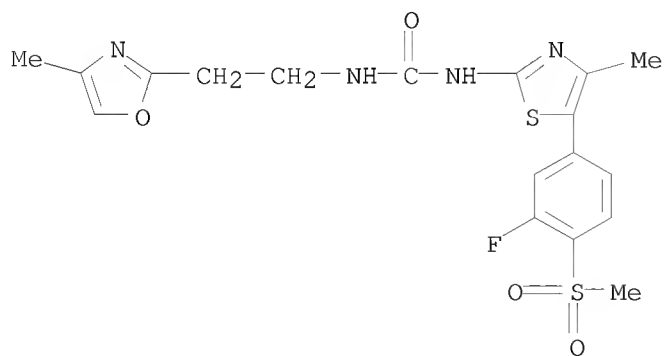
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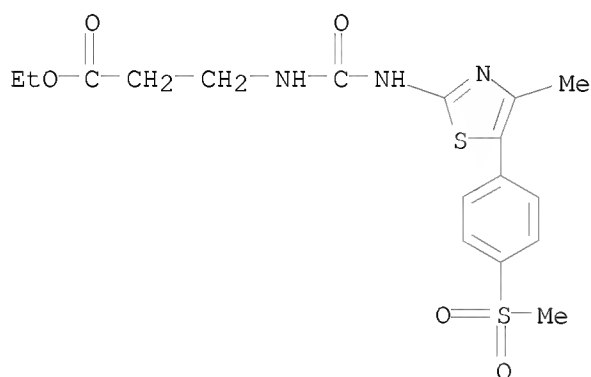


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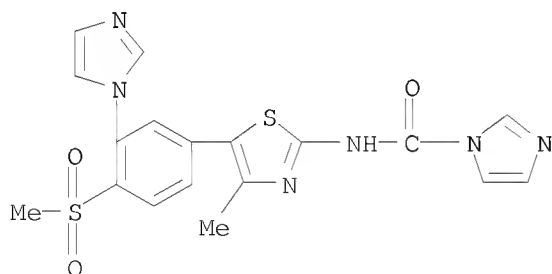
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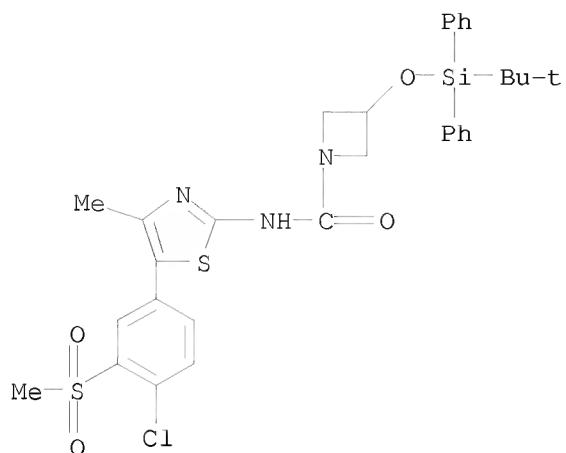
IT **593960-55-5P**, 3-[3-[5-[4-(Methanesulfonyl)phenyl]-4-methylthiazol-2-yl]ureido]propionic acid ethyl ester **593960-64-6P**, Imidazole-1-carboxylic acid [5-[3-(imidazol-1-yl)-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide **593960-67-9P**, 3-[(tert-Butyldiphenylsilyl)oxy]azetidine-1-carboxylic acid [5-[4-chloro-3-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide **593960-79-3P**, Imidazole-1-carboxylic acid [5-[3-fluoro-4-(methanesulfonyl)phenyl]-4-methylthiazol-2-yl]amide
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of phenylthiazole derivs. as phosphatidylinositol 3-kinase inhibitors)
 RN 593960-55-5 ZCAPLUS
 CN β -Alanine, N-[[[4-methyl-5-[4-(methylsulfonyl)phenyl]-2-thiazolyl]amino]carbonyl]-, ethyl ester (CA INDEX NAME)



RN 593960-64-6 ZCAPLUS
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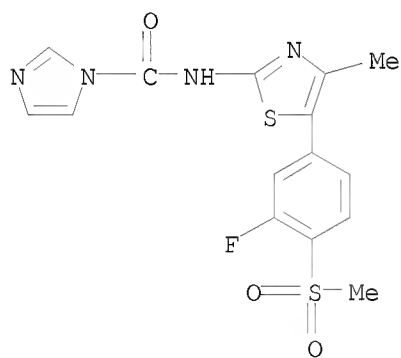


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RN 593960-79-3 ZCAPLUS

CN 1H-Imidazole-1-carboxamide, N-[5-[3-fluoro-4-(methylsulfonyl)phenyl]-4-methyl-2-thiazolyl]- (CA INDEX NAME)



REFERENCE COUNT:

14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT